

A simple analysis of the interband absorption coefficient of bulk and quantum well of nonparabolic semiconductors with application to $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ material

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A simple generalized theoretical analysis is presented for the calculation of interband optical absorption coefficient (IOAC) in bulk and quantum well structure of nonparabolic semiconductors, away from band edges. Consideration is taken of the dependence of wave-vector (\vec{k}) in the three energy band model of Kane. It has been found, taking $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ as example, that the IOAC for quantum wells (QWs) increases in steps with increasing photon energy which reflects the modification of band structure due to quantum confinement effect. It is also observed that IOAC in quantum wells (QWs) is largely dependent on the polarization of the light vector and on the well dimensions too. The effects of temperature and alloy composition dependence are also discussed. The analysis takes into account the effect of band mixing, and the expressions of the IOAC presented in this paper can easily be extended to include the effects of different external conditions, like strain, electric and magnetic fields. It has also been found that the contribution of the heavy hole valence band to IOAC in QW is more significant at positions near the band edge for polarization along the plane of the well and negligible along the well axis.

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1. Introduction

The interband optical absorption coefficient (IOAC) in semiconductor, being dependent on the DOS and on band profile, provides justification of many of the observed enhanced properties of quantum wells (QWs) and helps to describe the underlying theory of the optical interaction phenomena in semiconducting materials. Besides, this is related to various physical conditions like the relative dielectric constant, mechanical strain, and external fields etc. Extensive theoretical [1-4,6-9] and experimental [4,5,7] studies have been made for the determination of IOAC in bulk as well as QW structures of different semiconducting materials, due to its long standing interests in optoelectronics, for last few decades.

Specifically Quantum well (QW) structures have been under intensive investigation recently because of their potential applications in improving the optoelectronic device characteristics and uncovering new physical phenomena in both microscopic and macroscopic properties of the materials due to quantum confinement of carriers and related band modulation. Quantum-well lasers with ultrathin active layers [10], [11] have been found to have superior characteristics, such as ultralow threshold

current [12] - [16], less temperature dependence [17] and narrow gain spectrum [18]. The reasons for these improvements are confinement of electrons and holes and the change of densities of states (DOS). The quantization of the energy levels have also made it possible to realize a few new optoelectronic devices, e.g., Stark effect modulator [19] and intersubband absorption detectors [20-22].

However, such studies are made on the basis of the simplified assumption that the optical matrix element (OME) is constant with respect to the electron wave vector (\vec{k}), which is effective only for parabolic symmetrical band structure. It is also noted in [7] that the experimental curve differs significantly from the theoretical curve at high frequencies at which electrons are transferred deep into the conduction band. This deviation can be explained when the nonparabolicity of the energy band and the k -dependence of the cell-periodic functions are both taken into account [7]. In [23], for the first time, the IOAC in III-V, ternary and quaternary compounds has been investigated by considering the (\vec{k})-dependence of the OME for the bulk materials, without taking into account the heavy hole contribution. Nevertheless, it

appears from the literature that the IOAC of QW of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ material has yet to be investigated considering the (\vec{k}) dependent OME.

In this paper, we theoretically analyze the IOAC of the bulk and QW of small-gap nonparabolic materials whose energy band dispersion relations obey the widely accepted three energy band model of Kane and thereby consideration is taken of the wavevector (\vec{k}) -dependence on OME. We first derive the OME for bulk materials exhaustively which is slightly different from the expression given in [23] because they have not considered the electron spin conservation separately as the electrons take their transitions to different sublevels of conduction band as a result of interaction with photon of specific polarization and therefore it fails to explain the experimental results of polarization dependence of absorptions observed in QW structures. In our analysis of the OME we have taken into account the momentum and spin conservation separately and then calculated the transition probability that gives the complete wave function formalism for the OME. It duly incorporates the effect of band nonparabolicity and wave vector dependence of OME. The analytical formulation is then applied in the case of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ material for numerical illustration and experimental verification.

In this context it may be worth mentioning that the ternary alloy $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ is a classic narrow gap compound and is an extremely important optoelectronics material with novel characteristics. The band gap of this ternary alloy can be adjusted to cover the spectral range from 0.8 to over 30 nm by varying the alloy composition [23, 24] and attracted considerable interests in recent past. $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ finds extensive applications in infrared detector materials and photovoltaic detector arrays [25].

In section 2 of this article we have tried to develop a generalized formulation of IOAC for small band gap semiconducting materials the three band energy model of Kane and have then extended the formulation for QW structure of these materials. In this formulation we have duly incorporated the effect of band nonparabolicity,

specific of these kinds of materials and dependence of light polarization on interband optical absorption.

2. Formulation of the generalized IOAC for bulk materials

Light of proper energy greater than the band gap of the material excites the electrons from the valence band to conduction band, but their transition through absorption of light photon must depend on the structure of energy band and light polarization as well. If the rate of transitions per unit volume be $T(\omega)$ and the incident radiation intensity be $I(\omega)$, then the IOAC (Ξ) can, in general, be written as [7]

$$\Xi = \frac{\hbar\omega}{I(\omega)} T(\omega) \quad (1)$$

where $\hbar = h / (2\pi)$, h is the Plank constant and ω is the angular frequency of the incident radiation. Intensity of incident radiation is $I(\omega) = (1/2)Cn_r \epsilon_0 \omega^2 A_0^2$, where c is the velocity of light in free space, n_r is the relative refractive index of the semiconducting materials, ϵ_0 is the permittivity of free space, and A_0 is the amplitude of the incident light wave and can be expressed as $A_0^2 = 2\hbar / V_c n_r^2 \epsilon_0 \omega$, V_c being the volume of the crystal.

Transition rate $T(\omega)$ takes into account all the effects of band nonparabolicity, light polarization and the probability of allowed transitions and can be expressed in terms of OME as

$$T(\omega) = \frac{2\pi}{\hbar} \left(\frac{eA_0}{2m_0} \right)^2 \int \frac{2d^3k}{(2\pi)^3} \sum_i |\hat{a} \cdot p_{cvi}(\vec{k})|_{av}^2 \delta(E_c(\vec{k}) - E_{vi}(\vec{k}) - \hbar\omega) \quad (2)$$

where m_0 is the free electron mass, d^3k is the differential volume element in \vec{k} -space, \hat{a} is the polarization vector of the incident radiation, $\delta(\cdot)$ denotes the Dirac delta function and accounts for the selection condition for electron transition, $i = 1$ and 2 represents the light hole-split off band and heavy hole band respectively, $E_c(\vec{k})$ represents the energy of the conduction band (CB) with wave vector \vec{k} , $E_{vi}(\vec{k})$ represents the energy of the i -th valence

band (VB) with wave vector \vec{k} . $E_c(\vec{k}) - E_{vi}(\vec{k}) = \zeta_i(\vec{k}) = \zeta(\vec{k})$ (effective band gap $\zeta_i(\vec{k})$ may be treated as same for both the valence bands, the difference between them being negligible compared to the energy difference between the top of valence and the bottom of conduction band) denotes the \vec{k} -dependent energy difference between the corresponding VB and CB and $p_{cvi}(\vec{k})$ is the corresponding optical matrix elements (OME).

Incorporating expressions for A_0^2 , $I(\omega)$ and $T(\omega)$, Eq. (1) can be written as

$$\alpha = V_c \left(\frac{n_r}{c} \right) \left(\frac{2}{(2\pi)^3} \right) \frac{2\pi}{\hbar} \left(\frac{eA_0}{2m_0} \right)^2 \int d^3k \sum_i \left| \hat{a} \cdot p_{cvi}(\vec{k}) \right|_{av}^2 \delta(E_c(\vec{k}) - E_{vi}(\vec{k}) - \hbar\omega) \quad (3)$$

In k-p formalism, the energy eigen-values considering spin-orbit interaction of the electrons following Kane [6, 7, 9], three energy band model is

$$(E' - E_c)(E' - E_v)(E' - E_v + \Delta) - p^2 k^2 (E' - E_v + 2\Delta/3) = 0 \quad (4)$$

in which, $E' = E - \hbar^2 k^2 / 2m_0$, E is the energy eigen-value and is measured from the bottom of the conduction band minimum in vertically upward direction, m_0 is the free electron mass, E_c and E_v are the energies corresponding to the conduction band and valance band maximum, p is the momentum matrix element, \vec{k} is the electron wave vector and Δ is the spin-orbit splitting constant. Eliminating p , Eq. (4) simplifies as [9],

$$\frac{\hbar^2 k^2}{2m_c} \left(1 - \frac{m_c}{m_0} \right) = E' \left[\frac{(E_g + 2\Delta/3)(E' + E_g)(E' + E_g + \Delta)}{E_g(E_g + \Delta)(E' + E_g + 2\Delta/3)} \right] \quad (5)$$

m_c is the effective electron mass at the edge of the conduction band and is assumed isotropic near the band edge and E_g is the band gap. Thus, when, $\Delta \ll E_g$ and E or for large valence band split-off, Eq. (5) can be written as

$$E'(1 + \alpha E') = \frac{\hbar^2 k^2}{2m_c} \left(1 - \frac{m_c}{m_0} \right) \quad (6)$$

in which

$\alpha = (1/E_g)(1 - m_c/m_0)(1 - E_g\Delta/(3(E_g + 2\Delta/3)(E_g + \Delta)))$ is the non-parabolicity factor and in the limit of $\Delta \ll E_g$ it is $\approx 1/E_g$.

The effective energy difference between conduction and valence band at wave vector \vec{k} is then

$$\zeta(\vec{k}) = E_c(\vec{k}) - E_v(\vec{k}) = \left(E_g^2 + E_g \frac{\hbar^2 k^2}{m_r} \right)^{1/2} \quad (7)$$

in which E_g is the band-gap and m_r is the reduced mass and is given by $m_r^{-1} = m_c^{-1} + m_v^{-1}$, m_c the effective mass of the conduction band electron and m_v the effective mass of the heavy hole at the top of the valence band.

The doubly degenerate wave functions for the conduction band and light-hole band $u_1(\vec{k}, \vec{r})$ and $u_2(\vec{k}, \vec{r})$ can respectively be written as [9]

$$u_1(\vec{k}, \vec{r}) = [(is)\alpha'_1] a_{k_+} + \left[\frac{X' - iY'}{\sqrt{2}} \alpha'_2 \right] b_{k_+} + [Z'\alpha'_1] c_{k_+} \quad (8)$$

and

$$u_2(\vec{k}, \vec{r}) = [(is)\alpha'_2] a_{k_-} - \left[\frac{X' + iY'}{\sqrt{2}} \alpha'_1 \right] b_{k_-} + [Z'\alpha'_2] c_{k_-} \quad (9)$$

and the wave functions for heavy-hole bands $u_3(\vec{k}, \vec{r})$ and $u_4(\vec{k}, \vec{r})$ can respectively be [9]

$$u_3(\vec{k}, \vec{r}) = \left[\frac{X' - iY'}{\sqrt{2}} \alpha'_1 \right] \quad (10)$$

and

$$u_4(\vec{k}, \vec{r}) = \left[\frac{X' + iY'}{\sqrt{2}} \alpha'_1 \right] \quad (11)$$

where s is the s-type atomic orbital in both unprimed and primed coordinates, α'_1 indicates the spin down function in the primed coordinates. The coefficients of energy spectra for materials having large valence band split-off relative to band gap energy (i.e., $\Delta \ll E_g$, appropriate for $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ like materials) are [9],

$$a_{k_+} = \left(\frac{1 + \alpha E}{1 + 2\alpha E} \right)^{1/2}; \quad a_{k_-} = \left(\frac{\alpha E}{1 + 2\alpha E} \right)^{1/2} \quad (12)$$

$$b_{k+} = \left(\frac{1}{3} \cdot \frac{\alpha E}{1+2\alpha E} \right)^{1/2}; \quad b_{k-} = \left(\frac{1}{3} \cdot \frac{1+\alpha E}{1+2\alpha E} \right)^{1/2} \quad (13)$$

$$\begin{bmatrix} \alpha_2' \\ \alpha_1' \end{bmatrix} = \begin{bmatrix} e^{-i\phi/2} \cos \theta / 2 & e^{i\phi/2} \sin \theta / 2 \\ -e^{-i\phi/2} \sin \theta / 2 & e^{i\phi/2} \cos \theta / 2 \end{bmatrix} \begin{bmatrix} \alpha_2 \\ \alpha_1 \end{bmatrix} \quad (19)$$

$$c_{k+} = \left(\frac{2}{3} \cdot \frac{\alpha E}{1+2\alpha E} \right)^{1/2}; \quad c_{k-} = \left(\frac{2}{3} \cdot \frac{1+\alpha E}{1+2\alpha E} \right)^{1/2} \quad (14)$$

where X' , Y' , and Z' are the p-type atomic orbitals in the primed coordinates, α_2' indicates the spin-up function in the primed coordinates, E is the energy eigen value.

We can, therefore, write the expression for the OME as

$$OME = p_{cvi}(\vec{k}) = \langle u_1(\vec{k}, \vec{r}) | \bar{p} | u_{i2}(\vec{k}, \vec{r}) \rangle \quad (15)$$

where for index $i=1$, $i2=2$ and for $i=2$, $i2=3$ and 4 corresponds to electron transition from light hole band to conduction band heavy hole band to conduction band respectively. Intersubband transitions have not taken into account as they are not initiated by photon-electron interaction solely. One can therefore write

$$\langle S | \bar{p} | S \rangle = \langle X | \bar{p} | X \rangle = \langle Y | \bar{p} | Y \rangle = \langle Z | \bar{p} | Z \rangle = 0 \quad (16)$$

and

$$\langle X | \bar{p} | Y \rangle = \langle Y | \bar{p} | Z \rangle = \langle Z | \bar{p} | X \rangle = 0 \quad (17)$$

while for electron transition from VB to CB and we may write

$$\begin{aligned} \langle S | P | X \rangle &= \hat{i} \cdot \bar{p}_x; \quad \langle S | P | Y \rangle = \hat{j} \cdot \bar{p}_y; \\ \langle S | P | Z \rangle &= \hat{k} \cdot \bar{p}_z \end{aligned} \quad (18)$$

where \hat{i} , \hat{j} and \hat{k} are the unit vectors along the crystallographic axes. To account for the momentum conservation one has to rotate the axis in the plane of momentum vector (\vec{k}), then

$$\begin{aligned} \left| \langle \hat{a} \cdot p_{cvi}(\vec{k}) \rangle \right|_{av}^2 &= \frac{1}{4} P_z^2 \{M(\vec{k})\}^2 \int_0^{2\pi} \int_0^\pi \sin^3 \theta d\theta d\phi + \frac{1}{2} P_z^2 \{N(\vec{k})\}^2 \int_0^{2\pi} \int_0^\pi \cos^2 \theta \sin \theta d\theta d\phi \\ &= \frac{2\pi}{3} P_z^2 \left[\{M(\vec{k})\}^2 + \{N(\vec{k})\}^2 \right] \end{aligned} \quad (24)$$

and

$$\begin{bmatrix} X' \\ Y' \\ Z' \end{bmatrix} = \begin{bmatrix} \cos \theta \cos \phi & \cos \theta \sin \phi & -\sin \theta \\ -\sin \theta & \cos \phi & 0 \\ \sin \theta \cos \phi & \sin \theta \sin \phi & \cos \theta \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} \quad (20)$$

Incorporating the above mathematical formulation the average value of OME is then [23, 26]

$$\begin{aligned} p_{cvi}(\vec{k}) &= \langle u_1(\vec{k}, \vec{r}) | \bar{p} | u_2(\vec{k}, \vec{r}) \rangle \\ &= \frac{P}{\sqrt{2}} (b_{k+} a_{k-} \langle \alpha_2' | \alpha_2' \rangle - a_{k+} b_{k-} \langle \alpha_1' | \alpha_1' \rangle) (i\hat{r}_1 - \hat{r}_2) \\ &\quad + iP (c_{k+} a_{k-} + a_{k+} c_{k-}) \hat{r}_3 \langle \alpha_1' | \alpha_2' \rangle \end{aligned} \quad (21)$$

in which

$$P = \langle S | P | X \rangle = \langle S | P | Y \rangle = \langle S | P | Z \rangle = p_{cvi}(0),$$

the value at the band edge. Thus $p_{cvi}(0) = \int u_c^*(0, \vec{r}) P u_{v1}(0, \vec{r}) d^3 r$.

If a plane polarized light wave with polarization vector $\hat{a} = \hat{k}$ be incident, then we can write [26]

$$\langle \hat{a} \cdot p_{cvi}(\vec{k}) \rangle = \frac{P}{2} \hat{a} \cdot (i\hat{r}_1 - \hat{r}_2) \hat{r}_3 \{M(\vec{k})\} + \frac{P}{2} (\hat{a} \cdot \hat{r}_3) (i\hat{r}_1 - \hat{r}_2) \{N(\vec{k})\} \quad (22)$$

where

$$\begin{aligned} M(\vec{k}) &= \frac{1}{\sqrt{2}} (b_{k+} a_{k-} + a_{k+} b_{k-}) \\ N(\vec{k}) &= (c_{k+} a_{k-} + a_{k+} c_{k-}) \end{aligned} \quad (23)$$

Thus

$$\left| \langle \hat{a} \cdot p_{cvi}(\vec{k}) \rangle \right|^2 = \frac{1}{4} P_z^2 \sin^2 \theta \{M(\vec{k})\}^2 + \frac{1}{4} P_z^2 \cos^2 \theta \{N(\vec{k})\}^2$$

So the average value of $\left| \langle \hat{a} \cdot p_{cvi}(\vec{k}) \rangle \right|^2$ for a plane polarized light wave over the entire angle is

where $P_Z^2 = \left| \left(\hat{a} \cdot p_{cv1}(0) \right) \right|^2$ and

$$\left| \left(\hat{a} \cdot p_{cv}(0) \right) \right|^2 = \frac{m_0^2 E_g (E_g + \Delta)}{4m_r (E_g + 2\Delta/3)} \quad (25)$$

Proceeding in the similar manner the optical matrix element for the heavy hole would be,

$$p_{cv2}(\vec{k}) = \frac{P}{\sqrt{2}} \left(a_{k-} \langle \alpha_2 | \alpha_2 \rangle - a_{k+} \langle \alpha_1 | \alpha_1 \rangle \right) (i\hat{r}_1 - \hat{r}_2) = \frac{P}{2} (i\hat{r}_1 - \hat{r}_2) \hat{r}_3 \{ L(\vec{k}) \} \quad (26)$$

in which we denote, $L(\vec{k}) = \frac{1}{\sqrt{2}} (a_{k-} + a_{k+})$.

Therefore, one can obtain for plane polarized light with polarization vector $\hat{a} = \hat{k}$,

$$\left| \left(\hat{a} \cdot p_{cv2}(\vec{k}) \right) \right|_{av}^2 = \frac{1}{4} P_Z^2 \{ L(\vec{k}) \}^2 \int_0^{2\pi} d\phi \int_0^\pi \sin^3 \theta d\theta = \frac{2\pi}{3} P_Z^2 \{ L(\vec{k}) \}^2 \quad (27)$$

Replacing the coefficients of VB and CB wave functions from Eqs. (12) - (14) one can write

$$\left| \left(\hat{a} \cdot p_{cv1}(\vec{k}) \right) \right|_{av}^2 = \frac{2\pi}{3} \times \frac{m_0^2 E_g (E_g + \Delta)}{4m_r (E_g + 2\Delta/3)} \times \frac{5}{6} = \frac{5\pi}{9} \cdot \frac{m_0^2 E_g (E_g + \Delta)}{4m_r (E_g + 2\Delta/3)} \quad (28)$$

and (26) can be expressed as

$$\left| \left(\hat{a} \cdot p_{cv2}(\vec{k}) \right) \right|_{av}^2 = \frac{2\pi}{3} \times \frac{m_0^2 E_g (E_g + \Delta)}{4m_r (E_g + 2\Delta/3)} \times \frac{1}{2} \left\{ 1 + \frac{2\sqrt{(1+\alpha E)(\alpha E)}}{(1+2\alpha E)} \right\} \quad (29)$$

which after some algebraic manipulation further reduces to

$$\left| \left(\hat{a} \cdot p_{cv2}(\vec{k}) \right) \right|_{av}^2 = \frac{\pi}{3} \cdot \frac{m_0^2 E_g (E_g + \Delta)}{4m_r (E_g + 2\Delta/3)} \left\{ 1 + \frac{\sqrt{(\zeta(\vec{k})^2) - (E_g^2)}}{\zeta(\vec{k})} \right\} \quad (30)$$

The expression for interband optical absorption coefficient (IOAC) considering both light hole and heavy hole contributions can be written as,

$$\Xi_{bulk,l+h} = \frac{G_{bulk}}{3} \sqrt{(\hbar\omega)^2 - (E_g)^2} + \frac{G_{bulk}}{8\hbar\omega} \left((\hbar\omega)^2 - (E_g)^2 \right) \quad (31)$$

where,

$$G_{bulk} = \frac{2e^2}{3\hbar^2 c n_r \epsilon_0} \cdot \left(\frac{m_r}{E_g} \right)^{1/2} \cdot \frac{(E_g + \Delta)}{(E_g + 2\Delta/3)}.$$

3. Formulation of the generalized IOAC for quantum well (QW)

In QW structures the quantum confinement of electrons in one dimension modifies the density of states and removes the degeneracy of the electron energy bands that changes drastically the absorption coefficient. Here we have assumed the 2-D electron gas confined in the Z-direction interacted with polarized light. The IOAC is then

$$\Xi_{well} = A_c \left(\frac{n_r}{c} \right) \left(\frac{2}{(2\pi)^2} \right) \frac{2\pi}{\hbar} \left(\frac{eA_0}{2m_0} \right)^2 \times \int d^2k_t \sum_i \left\langle \left| \hat{a} \cdot p_{cvi}(\vec{k}) \right|^2 \right\rangle_{av} \delta(E_{cn}(\vec{k}) - E_{vni}(\vec{k}) - \hbar\omega) \quad (32)$$

where k_t is the in-plane wave vector and,

$$\zeta_n(\vec{k}) = E_{cn}(\vec{k}) - E_{vn}(\vec{k}) = \left(E_g^2 + E_g \frac{2m_c \beta(E)}{m_r} \right)^{1/2} \quad (33)$$

is the energy difference between the VB and CB at different \vec{k} values.

Here

$$\beta(E) = \frac{\hbar^2}{2m_c} k_t^2 + \frac{\hbar^2}{2m_c} \left(\frac{n\pi}{d_z} \right)^2, \quad (34)$$

where again m_c represents the effective mass of electrons in the conduction band, assumed isotropic near the band edge and $\beta(E_n) = (\hbar^2 / 2m_c) (n\pi / d_z)^2$ accounts for the sublevels of CB.

The quantized energy levels of CB are

$$E_n = \frac{1}{2\alpha} \left[-1 + \sqrt{1 + \frac{2\alpha\hbar^2}{m_c} \left(\frac{n\pi}{d_z} \right)^2} \right] \quad (35)$$

It is worth noting that at the band edge, i.e. at $k_t = 0$,

$$\zeta_n(0) = E_{cn}(0) - E_{vn}(0) = \left(E_g^2 + E_g \frac{\hbar^2}{m_r} \left(\frac{n\pi}{d_z} \right)^2 \right)^{1/2} \quad (36)$$

rather than E_g .

For plane polarized light with polarization vector $\hat{a} = \hat{k}$, (parallel polarization), the average value of OME for light-hole-conduction band (LH-CB) optical transition would be,

$$\left| \left(\hat{a} \cdot p_{cv1}(\vec{k}) \right) \right|_{av}^2 = \frac{2\pi}{4} P_z^2 \left[\left\{ M(\vec{k}) \right\}^2 \sin^2 \theta + \left\{ N(\vec{k}) \right\}^2 2 \cos^2 \theta \right] \quad (37)$$

in which, θ is the angle between the polarization vector \hat{a} of the incident wave and the well axis.

Similarly, for heavy-hole-conduction band (HH-CB) OME can be written as,

$$\Xi_{well,l+h} = \sum_n \left\{ \frac{2G_{well} \sin^2 \theta}{3} + \frac{G_{well} \sin^2 \theta}{2} \left(\frac{\sqrt{(\zeta_n(\vec{k})^2) - \zeta_n(0)^2}}{\zeta_n(\vec{k})} \right) + \frac{4G_{well} \cos^2 \theta}{3} \right\} H(\hbar\omega - \zeta_n(0)) \quad (39)$$

where $G_{well} = \frac{\pi e^2}{8d_z \hbar c n_r \epsilon_0} \cdot \frac{(E_g + \Delta)}{(E_g + 2\Delta/3)}$, $H(\cdot)$ is the Heaviside step function and $\zeta_n(0)$ is given by Eq. (36).

$$\begin{aligned} \left| \left(\hat{a} \cdot p_{cv2}(\vec{k}) \right) \right|_{av}^2 &= \frac{1}{4} \sin^2 \theta P_z^2 \left\{ L(\vec{k}) \right\}^2 \int_0^{2\pi} d\phi \\ &= \frac{2\pi}{8} \cdot \frac{m_0^2}{4m_r} \cdot \frac{E_g(E_g + \Delta)}{(E_g + 2\Delta/3)} \sin^2 \theta \left(1 + \frac{\sqrt{(\zeta_n(\vec{k})^2) - \zeta_n(0)^2}}{\zeta_n(\vec{k})} \right) \end{aligned} \quad (38)$$

Thus, we finally arrive at the expression of total value of IOAC in QW for light with polarization vector $\hat{a} = \hat{k}$, (parallel polarization), as,

For plane polarized light with polarization vector $\hat{a} = \hat{i}$ or \hat{j} (perpendicular polarization), the expressions for OME would be

$$\left| \left(\hat{a} \cdot p_{cv1}(\vec{k}) \right) \right|_{av}^2 = \frac{2\pi}{4} P_z^2 \left[\left\{ M(\vec{k}) \right\}^2 \left(\frac{1 + \cos^2 \theta}{2} \right) + \left\{ N(\vec{k}) \right\}^2 \sin^2 \theta \right] \quad (40)$$

$$\left| \left(\hat{a} \cdot p_{cv2}(\vec{k}) \right) \right|_{av}^2 = \frac{2\pi}{8} P_z^2 \left(\frac{1 + \cos^2 \theta}{2} \right) \left(1 + \frac{\sqrt{(\zeta_n(\vec{k})^2) - \zeta_n(0)^2}}{\zeta_n(\vec{k})} \right) \quad (41)$$

corresponding to LH-CB and HH-CB optical transition, respectively. Finally, the total IOAC for light polarization vector $\hat{a} = \hat{i}$ or \hat{j} , (perpendicular polarization), is given by

$$\begin{aligned} \Xi_{well,l+h} &= \sum_n \left\{ \frac{2G_{well}}{3} \left(\frac{1 + \cos^2 \theta}{2} \right) \right. \\ &\left. + \frac{G_{well}}{2} \left(\frac{1 + \cos^2 \theta}{2} \right) \left(\frac{\sqrt{(\hbar\omega)^2 - \zeta_n(0)^2}}{\hbar\omega} \right) + \frac{2G_{well}}{3} \sin^2 \theta \right\} H(\hbar\omega - \zeta_n(0)) \end{aligned} \quad (42)$$

$$\begin{aligned} E_g(x) &= [-0.302 + 1.93x + 5.25 \times 10^{-4} T(1-2x) - 0.810x^2 + 0.832x^3] \text{eV}; \\ \Delta &= (0.63 + 0.24x - 0.27x^2) \text{eV}; m_c = 3\hbar^2 E_g(x) [4t^2(x)]^{-1}, t(x) = [(\hbar^2 / 2m_0)(18 + 3x)]^{1/2}; \\ m_v &= 0.4m_0, n_r = 3.56; x = 0.2 - 0.6; \end{aligned}$$

we have calculated the IOAC as a function of incident photon energy $\hbar\omega$ (in eV), which is shown in Fig. 1. Here the curves labeled 'light-hole' and 'light-hole +heavy-

hole' represent the IOAC considering only light-hole dependence and both the heavy-hole and light-hole dependence, respectively. The IOAC increases with

increasing incident photon energy and the separation between the two curves also increases. Besides that, from the Fig. 1 it is clear that the influence of heavy hole is significant especially at high energy regimes and should be taken into consideration for the purpose of accurate evaluation of IOAC. It is also noteworthy that the total IOAC has a $\sqrt{(\hbar\omega)^2 - (E_g)^2}$ dependence near band edge and $\left((\hbar\omega)^2 - (E_g)^2\right)$ dependence at higher values of wave vector (\vec{k}), in contrast to the conventional idea of $\sqrt{\hbar\omega - E_g}$ dependence on $\hbar\omega$. This is due to the effect of nonparabolicity in the band structure of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$.

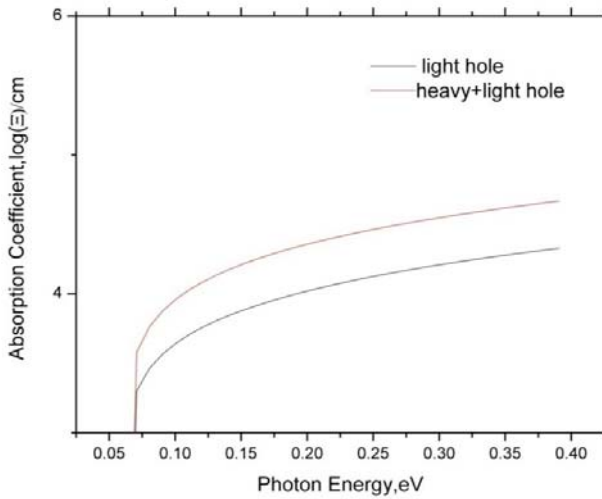


Fig. 1. The plot of IOAC in bulk $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ as a function of incident photon energy $\hbar\omega$ (in eV).

In Fig. 2, we have plotted absorption coefficient (IOAC) for different polarization directions of the incident light vectors as a function of photon energy for QW of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ material. In the plot both the curves (a) and (b) represent the total IOAC taking into account of heavy-hole and light-hole contributions where curve (a) represents the z-polarized light (parallel polarization) and (b) represents the x or y-polarized light (perpendicular polarization) assuming the width of the QW as $L=40$ nm in the z-direction. It is observed that in QW above the $\zeta_n(0)$, at same incident photon energy the IOAC value for parallel polarization (z- polarization) is higher in magnitude than that for perpendicular polarization (x or y-polarization).

Besides, it is observed that the IOACs increase in steps for both parallel polarization and perpendicular polarization with increasing photon energy. This is due to the fact that with increasing photon energy electrons are transferred to higher sublevels of CB. Comparing the shape of the curves (a) and (b) it also appears that only light-hole band contributes to the absorption for incident

light polarization in the z direction while both light-hole and heavy-hole band contribute for light polarization in the x-y plane. For lower photon energies the light-hole contribution is much smaller near band edges as depicted by the curved variation due to heavy hole. However, as the photon energies increased the contribution light-hole electrons become increasingly important compared to heavy-hole. It is worth mentioning that the foregoing theoretical results agree well with the experimental results provided in [5] and hence is an indirect test of the validity of our theoretical results.

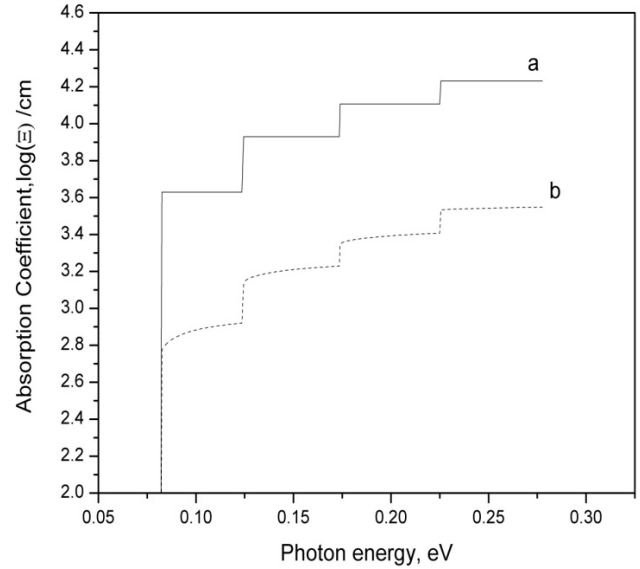


Fig. 2. The plot of IOAC in QW of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ as a function of incident photon energy $\hbar\omega$ (in eV), for $\theta=0^\circ$, and for (a) light polarization vector along z-direction (b) light polarization vector along x or y-direction.

In Figs. (3) and (4), the influence of temperature and alloy composition are presented for polarization in the z direction, respectively. It is observed that the energy gap between valence and conduction band being dependent on temperature the chief effect of increasing temperature is the shift of photon energies for a given absorption, due to the change in the $\zeta_n(0)$ value (eq. (36)). However, as band structure is largely dependent on alloy composition in terms of variation of band gap energy (E_g), spin-orbit splitting (Δ) and the effective mass in the conduction band (m_c) etc., then with less amount of Hg in alloy composition increases the photon energy requirement for a given absorption. The value of absorption coefficient also decreases by reducing Hg composition. Although we have presented plots for a polarization in z- direction, the similar results can easily be obtained for polarization in x-y plane also. It should be noted that the variation of IOAC with respect to change in well dimensions can also be evaluated easily from these formulations, as the effect of

reducing well dimension removes the band degeneracy further and that increases IOAC at higher photon energies.

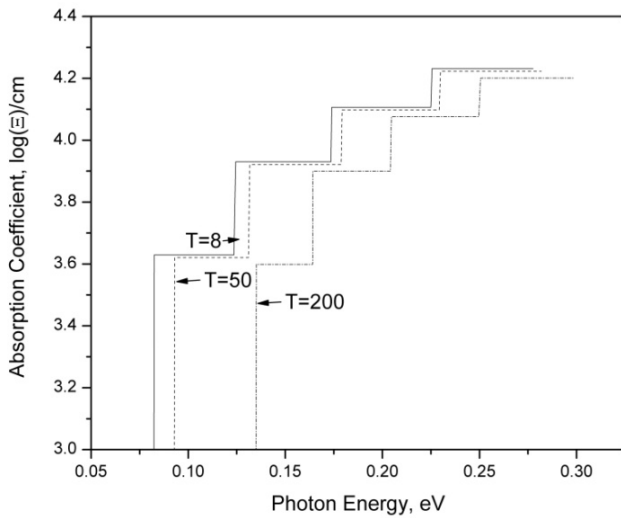


Fig. 3. Variation of IOAC with respect to temperature (T) in QW of $Hg_{1-x}Cd_xTe$ as a function of incident photon energy $\hbar\omega$ (in eV), for $\theta=0^\circ$, and for the case of light polarization vector along z -direction.

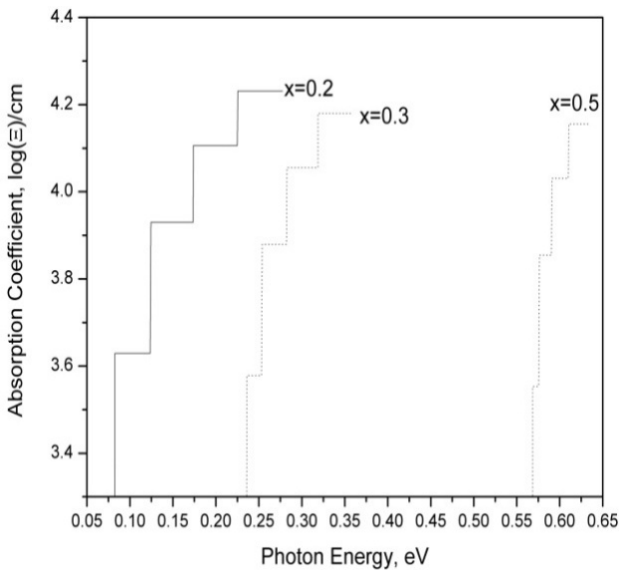


Fig. 4. Variation of IOAC with respect to alloy composition (x) in QW of $Hg_{1-x}Cd_xTe$ as a function of incident photon energy $\hbar\omega$ (in eV), for $\theta=0^\circ$, and for the case of light polarization vector along z -direction.

5. Conclusion

A simple theory of IOAC for nonparabolic material is developed considering the wave vector dependence of the energy band structure. The analysis includes the general formulation of IOAC in bulk and QW of low band gap semiconducting materials considering both the heavy-hole and light-hole contributions. It is found that the IOAC for

the bulk is proportional to $\sqrt{(\hbar\omega)^2 - (E_g)^2}$ near band edge and $\left((\hbar\omega)^2 - (E_g)^2\right)$ for high values of wave vector (\vec{k}), unlike the conventional idea of $\sqrt{\hbar\omega - E_g}$ dependence on incident photon energy. It is also observed that the IOAC is strongly influenced by the direction of polarization vector of incident light in QW. The reduction of dimensions of QW increases the absorptions for a given sub-band. The absorption in $Hg_{1-x}Cd_xTe$ and like material is found to follow these formulations of IOAC. Besides, the influences of temperature and alloy compositions are studied within this formulation.

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